The QCDOC Computer: From Design to First Results

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Columbia University
RBC Collaboration

Dedication of the US DOE QCDOC Computer
Brookhaven National Laboratory
November 30, 2005

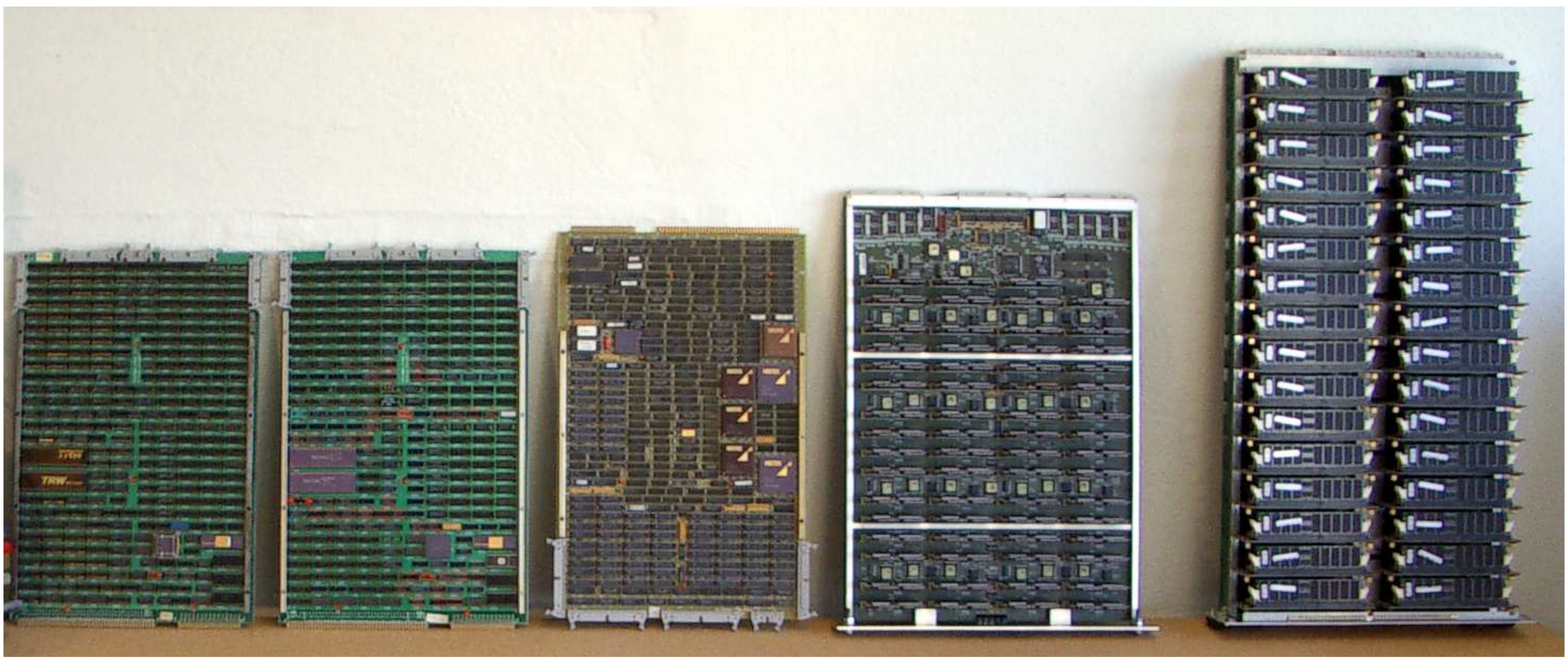
1. Some computer design from 1980's to present
2. Theoretical improvements in lattice QCD
3. If you build it, algorithms will come
4. Physics from QCDOC

Columbia University Designed Computers

Machine	Date	Processor (FPU precision)	Nodes	Speed (Gflops)	Memory (GBytes)
Intel x86 plus numeric co-processors, 2-d mesh, NN shared memory					
16-node	1985	286/TRW (22)	16	0.25	0.016
64-node	1987	286/Weitek (32)	64	1.0	0.128
256-node	1989	286/Weitek (64)	256	16.0	0.5
Digital signal processor based, 4-d mesh, bit-serial communication					
CU QCDSP	1998	TI DSP (32)	8,192	400	16
RBRC QCDSP	1998	TI DSP (32)	12,288	600	24
Power-PC based, 6-d mesh, bit-serial communication					
RBRC QCDOC	2005	440 PPC (64)	12,288	9,830	1,570
UKQCD QCDOC	2005	440 PPC (64)	12,288	9,830	1,570
US LGT QCDOC	2005	440 PPC (64)	12,288	9,830	1,570

Motherboards from Columbia University Computers

16-node	**64-node**	**256-node**	**QCDSP**	**QCDOC**
16 Mflops	16 Mflops	64 Mflops	3.2 Gflops	64 Gflops
1985	1987	1989	1998	2004
2-d mesh	2-d mesh	2-d mesh	4-d mesh	6-d mesh



QCDOC Design Group

- Columbia:

  Faculty: Norman Christ, Robert Mawhinney

  Postdoc: Azusa Yamaguchi

  Staff researcher: Zhihua Dong

  Student: Calin Cristian, Changhoan Kim, Xiaodong Liao, Guofeng Liu

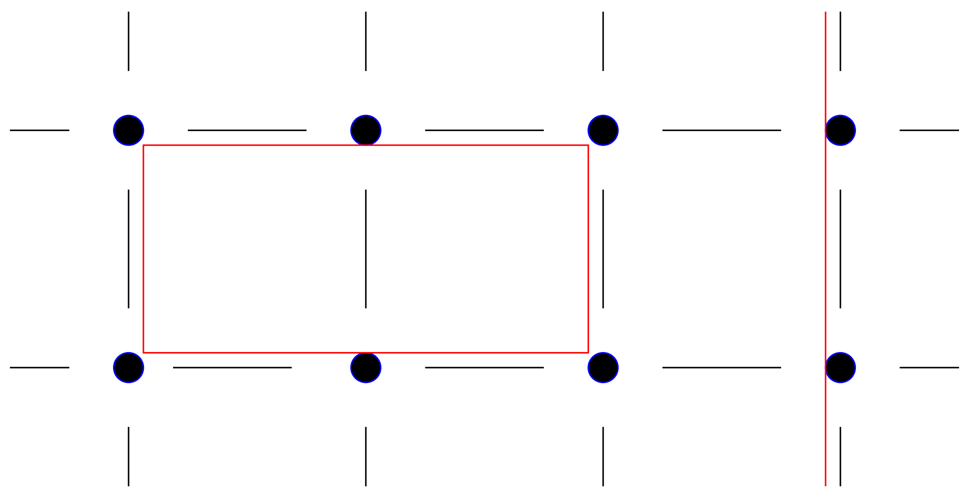
  New students: Saul Cohen, Meifeng Lin
- IBM: Dong Chen, Alan Gara
- RBRC: Shigemi Ohta, Tilo Wettig
- UKQCD: Peter Boyle, Balint Joo
- SciDAC: Chulwoo Jung, Kostantin Petrov

QCDOC Design Environment

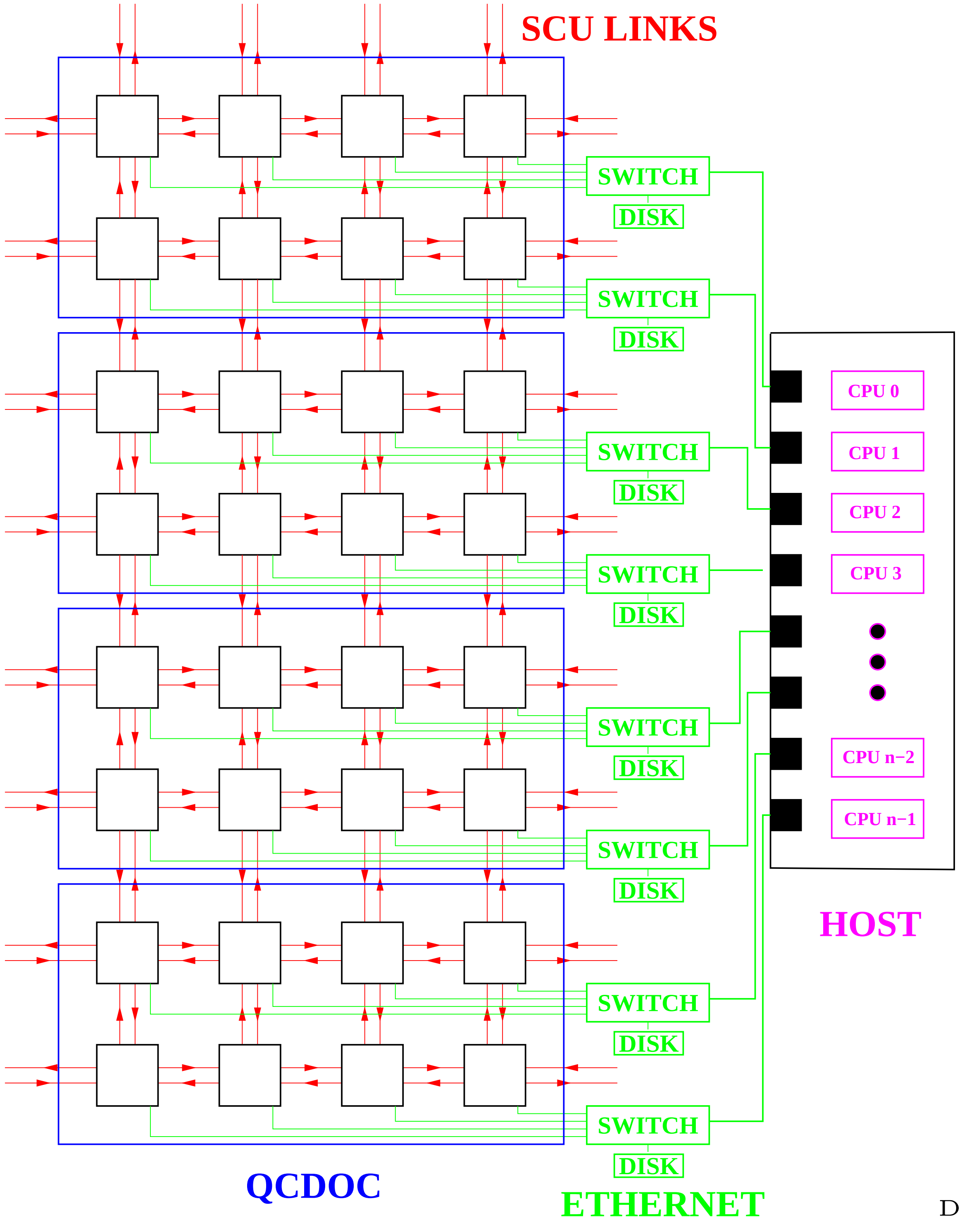
- Overall design was responsibility of design group centered at Columbia.
- R&D relationship with IBM Yorktown Heights
  - Gara led EDRAM team of Ben Nathanson and Minhua Lu
  - Electrical modeling support by Paul Coteus.
- External ASIC customer relationship with IBM Microelectronics Division
  - Harry Linzer, Beth Danford and Doan Trinh Nguyen at Raleigh did much to help with layout, timing and answering questions
  - Additional engineering support from IBM Rochester, MN.
- QCDOC research and development was supported by the U.S. Department of Energy, the RIKEN-BNL Research Center and the UKQCD collaboration through their PPARC grant.

QCDOC Overview

- Uses IBM's System-On-a-Chip Technology
- 64-bit, 0.8 Gflop Power PC 440 processor with L1 instruction and data caches.
- 4 MBytes embedded DRAM and 128 Mbytes external DDR SDRAM per node
- 100 Mbit Ethernet and 100 Mbit Ethernet/JTAG per node
- High-bandwidth (1.3 GBytes/sec), low-latency ($\approx$ 600 ns) 6-D nearest neighbor communications network.



- Low-electrical power ($\approx$ 8 watts/node) allows dense packing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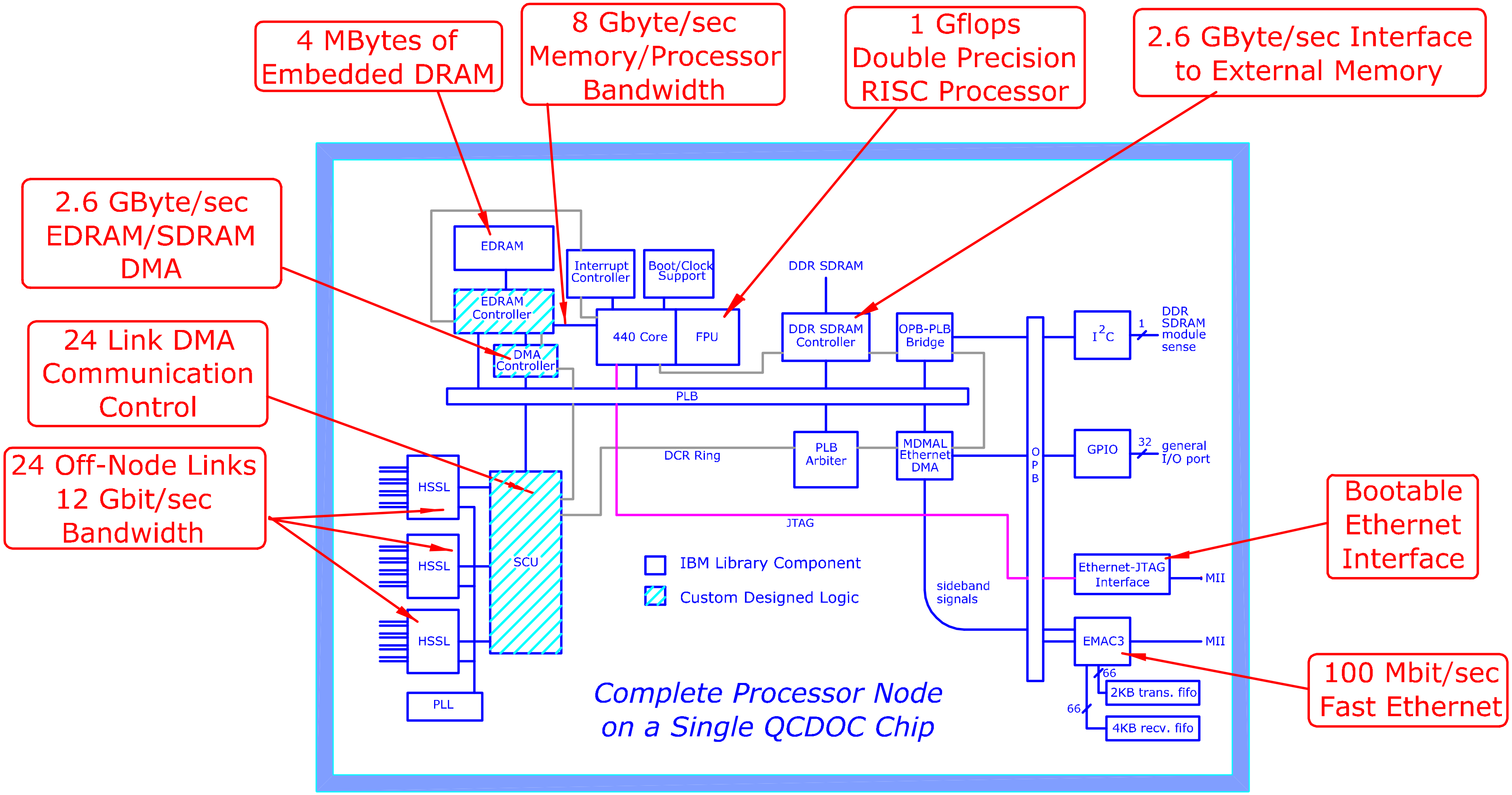
CPU 0
CPU 1
CPU 2
CPU 3
CPU n−2
CPU n−1
HOST
QCDOC
ETHERNET

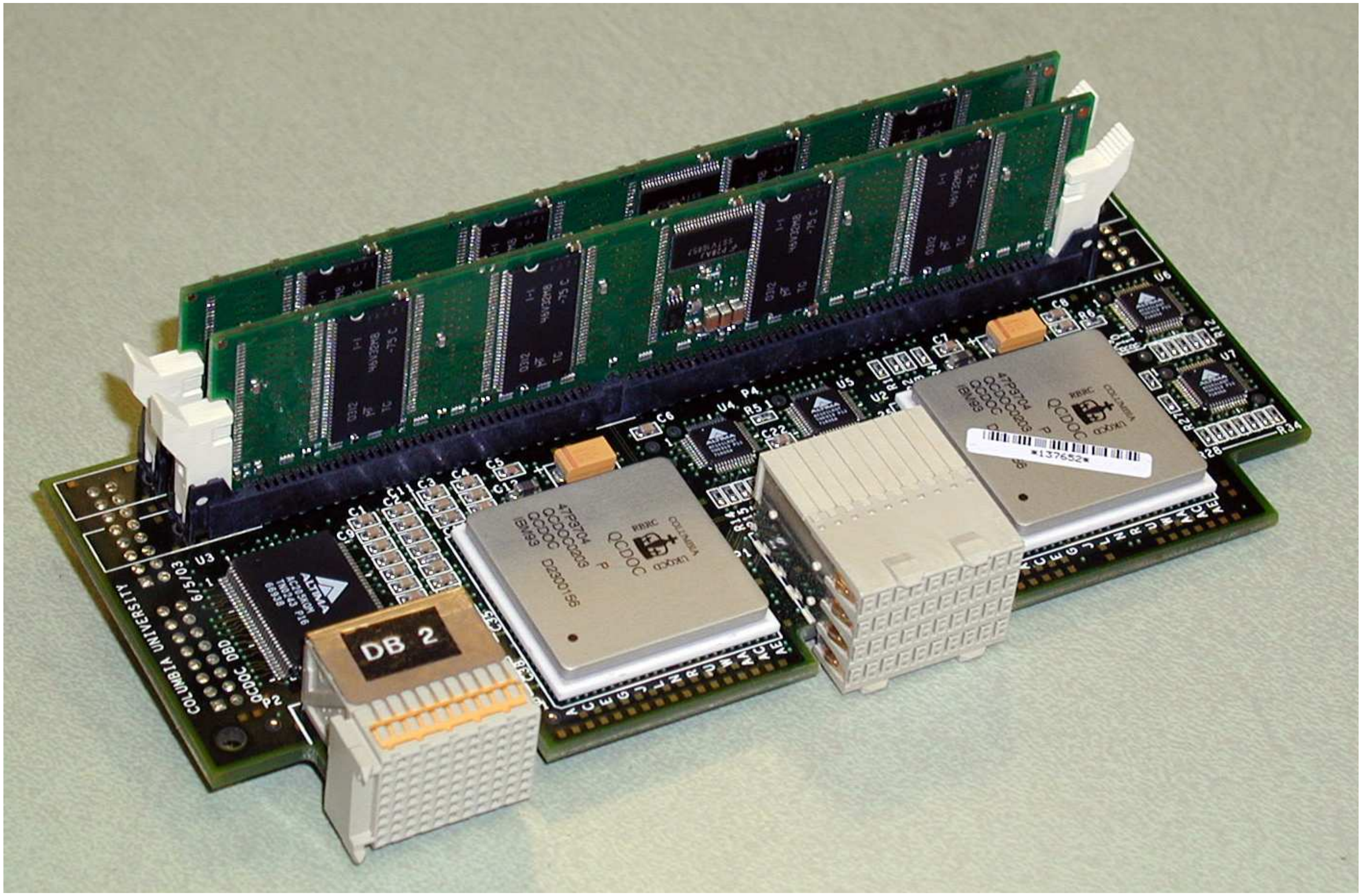
The QCDOC ASIC



QCDOC ASIC - First Prototypes at Columbia June 5, 2003

QCDOC Daughterboard - First Prototypes June 27, 2003

Major components are: 2 ASICs, 2 DDR SDRAM DIMMs and 5-port ethernet hub



QCDOC Software

- QCDOC operating system - QOS (Boyle, Joo, Petrov)
  - Boyle led software architecture design and wrote most of QOS
  - Boots, runs and helps debug QCDOC.
  - Unix-like user environment on each node, including file system access.
  - AIX host to achieve good I/O performance to QCDOC.
- Columbia Physics System (RBC and UKQCD collaborations)
  - Original C++ code for QCDSP ANSI-fied, ported to QCDOC
  - Also runs on clusters, but not performance tuned currently
  - Publicly available with version control managed by Chulwoo Jung
- QCDOC Software for other users
  - Optimized assembly kernels for Wilson and DWF (Boyle), staggered and ASQTAD (Cristian, Jung) and P4 staggered (Cheng) available
  - Batch queues being implemented (Stratos)
  - SciDAC QCD Message Passing (QMP) implemented by Jung

ASQTAD Performance

	Sites/ node	Optimized					MILC		
Precision		Single	Double				Single		Double
Machine size		1024	1024	sim	128	128	128	16	16
		CG		Dslash	Dslash	CG	CG	CG/QDP	CG
Asqtad.CG	2^4			43%	22%	19%		2%	
	4^4	44%	38%		42%	40%	9.5%	15%	7.5%
	6^4	44%	27%		36%	36%	13.6%	19%	8.6%
	8^4	34%	18%		28%	28%	12.3%		8.1%
Asqtad force	2^4	19%							
	4^4	35%					10.0%		6.1%
	6^4	29%					10.8%		6.1%
	8^4	20%					8.2%		6.0%
Asqtad/ Symanzik link products	2^4	23%							
	4^4	50%					7.2%		7.1%
	6^4	49%					8.1%		6.4%
	8^4	27%					8.5%		6.8%

Application Performance

(double precision)

1024-node machine:

Fermion action	Local volume	Dirac performance	CG performance
Wilson	2^4	44%	32%
Wilson	4^4	44%	38%
Clover	4^4	54%	47.5%
DWF	4^5	47%	42%
ASQTAD	4^4	40%	38%

4096-node machine (UKQCD):

DWF/24^3 x 64/RHMC	CG:	1.1 Tflops (34%)
(Local vol: 6x6x6x2x8)	Complete code:	0.97 Tflops (29%)

Lattice QCD More Complicated than Continuum

Continuum	Lattice
Gauge invariance	Gauge invariance
Lorentz invariance	Hypercube invariance
N_f quarks	Generally more than N_f quarks
Chiral symmetry broken by quark masses	Chiral symmetry broken by quark masses and lattice effects
θ observed small	Numerical simulations with non-zero θ not currently possible
Renormalization of operators simplified by full symmetry and mass-independent schemes	Breaking symmetries makes renormalization of operators difficult to virtually impossible

Improved Fermion Actions

	$SU_V(N_f)$	$SU_A(N_f)$	$U_V(1)$	$U_A(1)$
Wilson clover	$\surd$	$\times$ $\mathcal{O}(a^2)$	$\surd$	$\times$ $\mathcal{O}(a^2)$
ASQTAD staggered	$\times$ $\mathcal{O}(a^2)$ discrete subgroup	$\times$ $\mathcal{O}(a^2)$ $U(1)$ subgroup	$\surd$	$\times$ $\mathcal{O}(a^2)$
	($4N_f$ flavors on lattice from fermion doubling)			
domain wall	$\surd$	$\surd$ $\mathcal{O}\left(ae^{-\alpha L_s}\right)$	$\surd$	$\times$ $\mathcal{O}\left(ae^{-\alpha L_s}\right)$
	(for modes bound to 4-d walls)			

- Wilson clover fermions markedly improves chiral symmetry.
- ASQTAD staggered fermions have much smaller $\mathcal{O}(a^2)$ flavor breaking.
- DWF also gives off-shell improvement.

Domain Wall Fermion Operator

- Introduce extra dimension, labeled by s

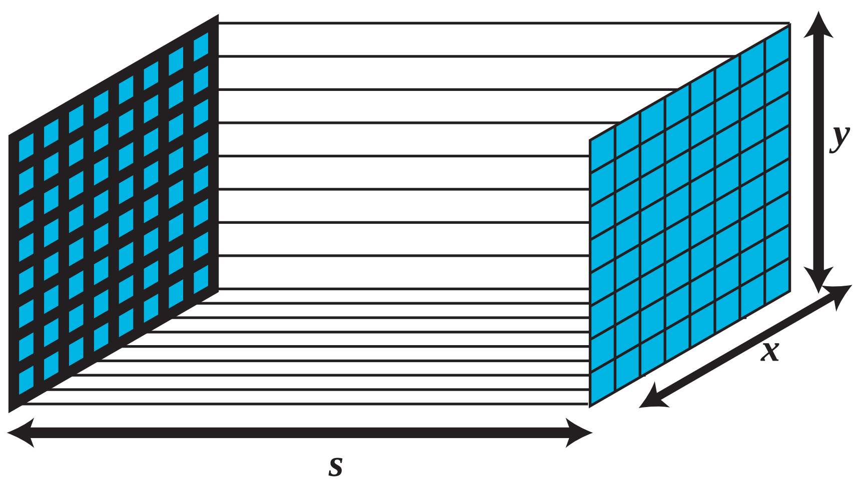
$$D_{x,s;x',s'} = \delta_{s,s'} D^{\parallel}_{x,x'} + \delta_{x,x'} D^{\perp}_{s,s'}$$

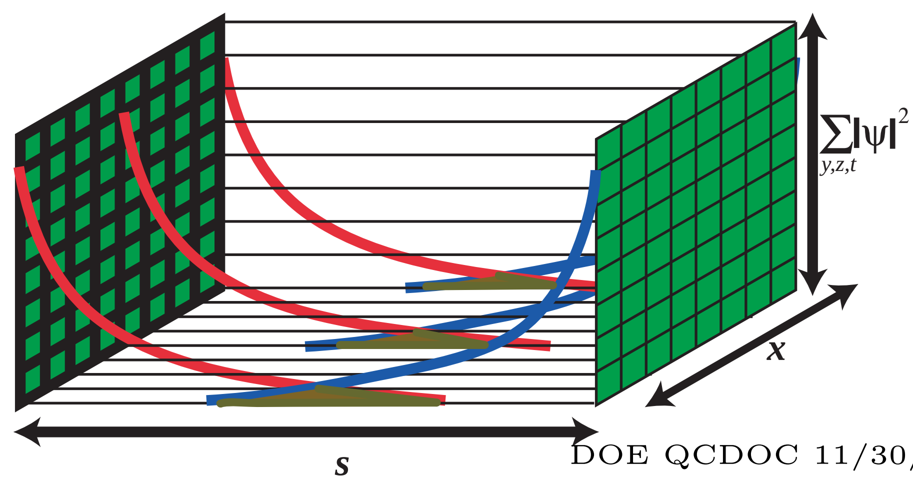
- $D^{\parallel}_{x,x'}$ is a Wilson Dirac operator with an opposite sign for the mass term.

$$D^{\parallel}_{x,x'} = \frac{1}{2} \sum_{\mu=1}^{4} \left[(1-\gamma_\mu) U_{x,\mu} \delta_{x+\hat{\mu},x'} + (1+\gamma_\mu) U^{\dagger}_{x',\mu} \delta_{x-\hat{\mu},x'} \right] + (M_5 - 4)\delta_{x,x'}$$

- $D^{\perp}_{s,s'}$ couples points in fifth dimension, distinguishing left and right handed fermions

$$\frac{1}{2} \left[(1-\gamma_5)\delta_{s+1,s'} + (1+\gamma_5)\delta_{s-1,s'} - 2\delta_{s,s'} \right] - \frac{m_f}{2} \left[(1-\gamma_5)\delta_{s,L_s-1}\delta_{0,s'} + (1+\gamma_5)\delta_{s,0}\delta_{L_s-1,s'} \right]$$





Lattice QCD Algorithms

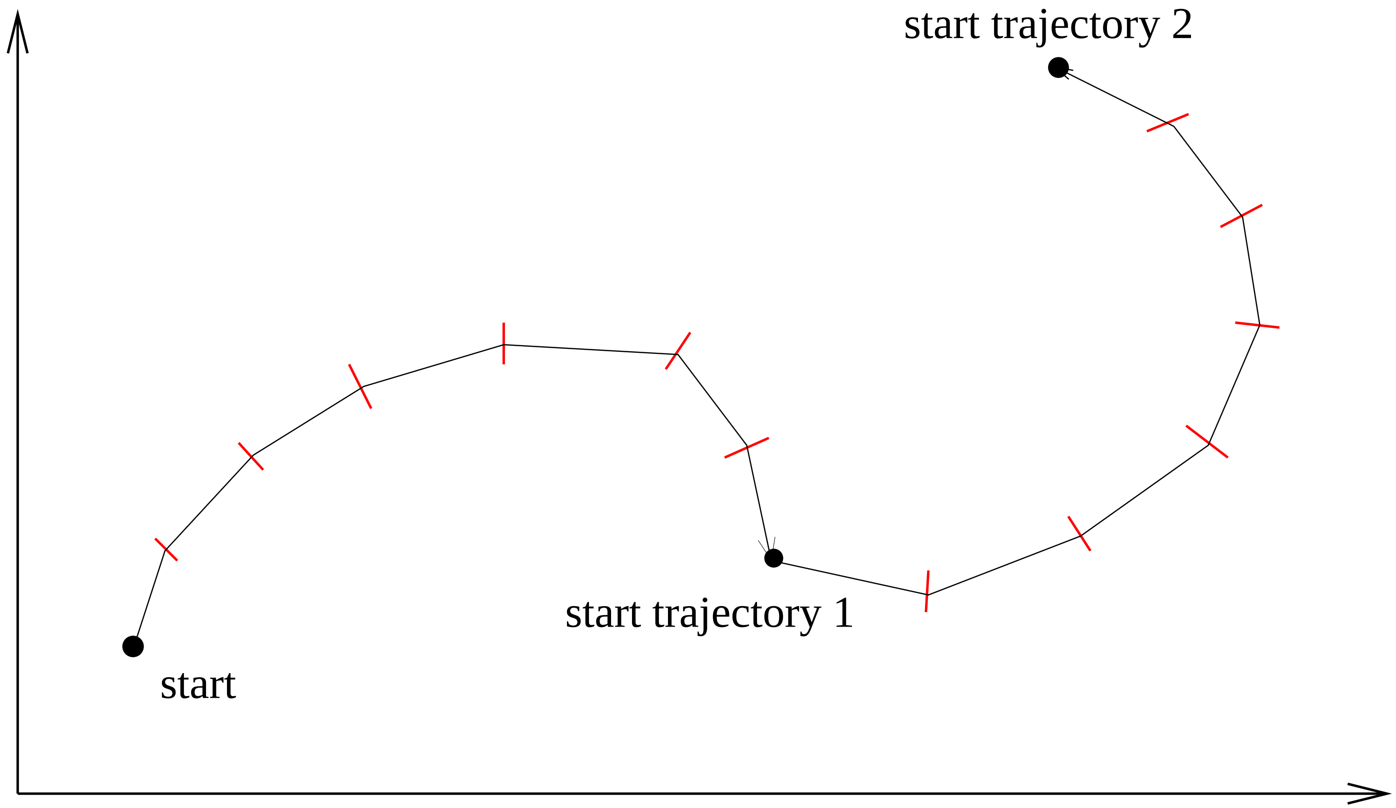
- Fermion determinant represented by "pseudo fermion" fields

$$
\begin{aligned}
Z &= \int [dU]\,[d\psi]\,[d\bar{\psi}]\,\exp\left\{-\beta S_g + \bar{\psi}(\not{D}+m)\psi\right\} = \int [dU]\,\det(\not{D}+m)\exp\left\{-\beta S_g\right\} \\
&= \int [dU]\,[d\phi^*][d\phi]\,\exp\left\{-\beta S_g + \phi^*(\not{D}+m)^{-1}\phi\right\} \\
&= \int [dU]\,[d\Pi]\,[d\phi^*][d\phi]\,\exp\left\{-\Pi^2 - \beta S_g + \phi^*(\not{D}+m)^{-1}\phi\right\} \\
&= \int [dU]\,[d\Pi]\,[d\phi^*][d\phi]\,\exp\left\{-\Pi^2 - \beta S_g + \phi^*[(\not{D}+m)(\not{D}^\dagger+m)]^{-1/2}\phi\right\}
\end{aligned}
$$

- Since $\det(\not{D}+m)$ is positive definite, it equals $\det[(\not{D}+m)(\not{D}^\dagger+m)]^{-1/2}$.
- All eigenvalues of $(\not{D}+m)(\not{D}^\dagger+m)$ are positive, which yields a positive definite probability weight for a single quark flavor.
- The Rational Hybrid Monte Carlo algorithm of Clark and Kennedy (UKQCD) is an exact algorithm that utilizes the square root.
- Therefore, 2+1 flavor DWF QCD can be simulated with an exact algorithm.

Moving Through the Phase Space of QCD

- RHMC implemented in CPS software for QCDOC
- Motion through phase space occurs in small steps
- What is efficiency for decorrelating gluon configurations?



RBRC-BNL-CU (RBC) Collaboration, July 2005

RBRC

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Izubuchi, Taku (Kanazawa)
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Jung, Chulwoo
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Soni, Amarjit

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Christ, Norman
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Li, Sam
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Loktik, Oleg
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UKQCD DWF Collaborators

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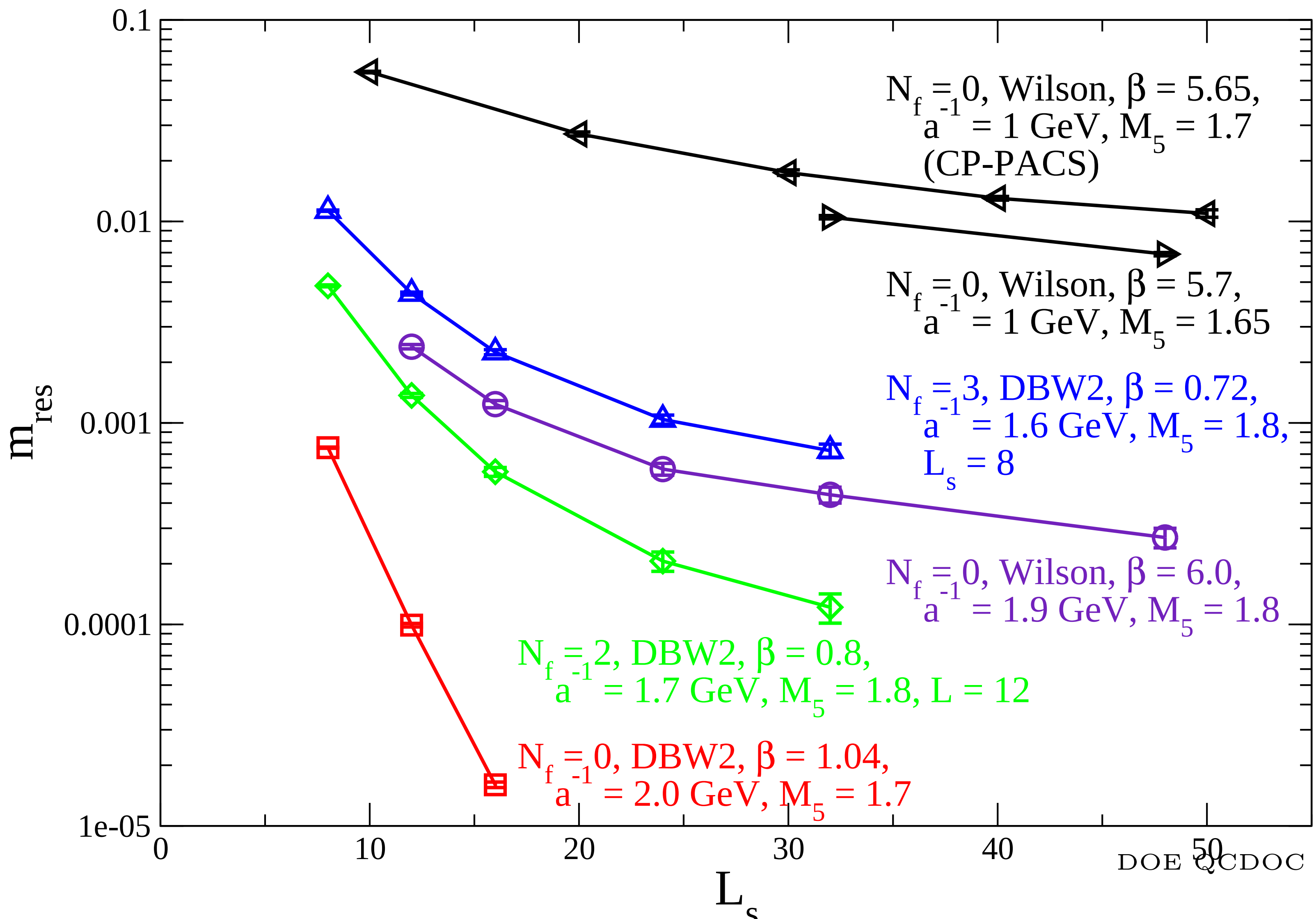
Kenway, R. D.
Maynard, C. M.
Tweedie, R. J.
Yamaguchi, A.

$m_{\rm res}$ versus L_s for $N_f = 0, 2$ and 3

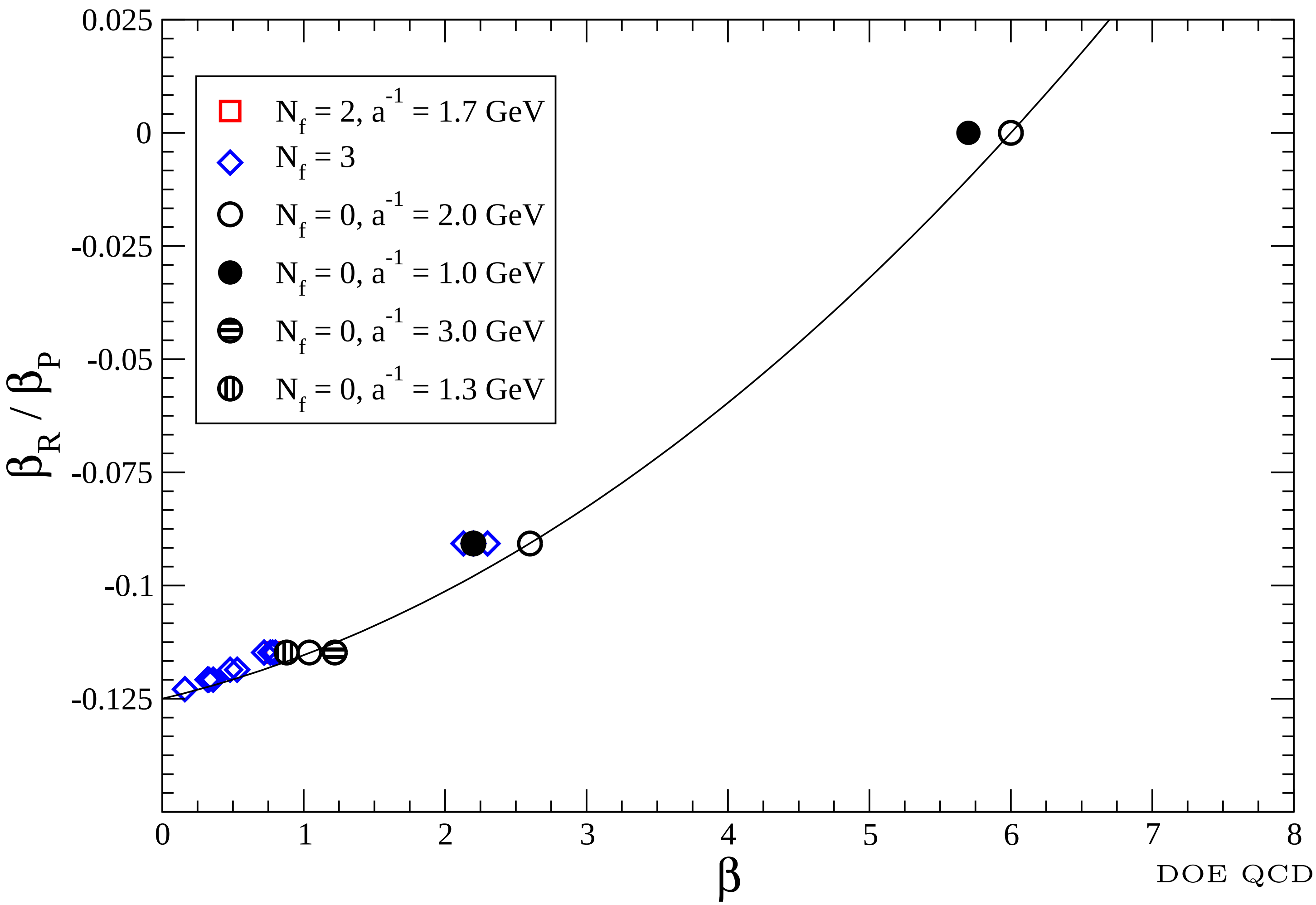
Compare gauge actions composed of plaquette and rectangle terms.

$$S_g = (\beta/3)\left\{(1-8c_1)\sum \mathrm{Re}(\mathrm{Tr}U_P) + c_1 \sum \mathrm{Re}(\mathrm{Tr}U_R)\right\}$$

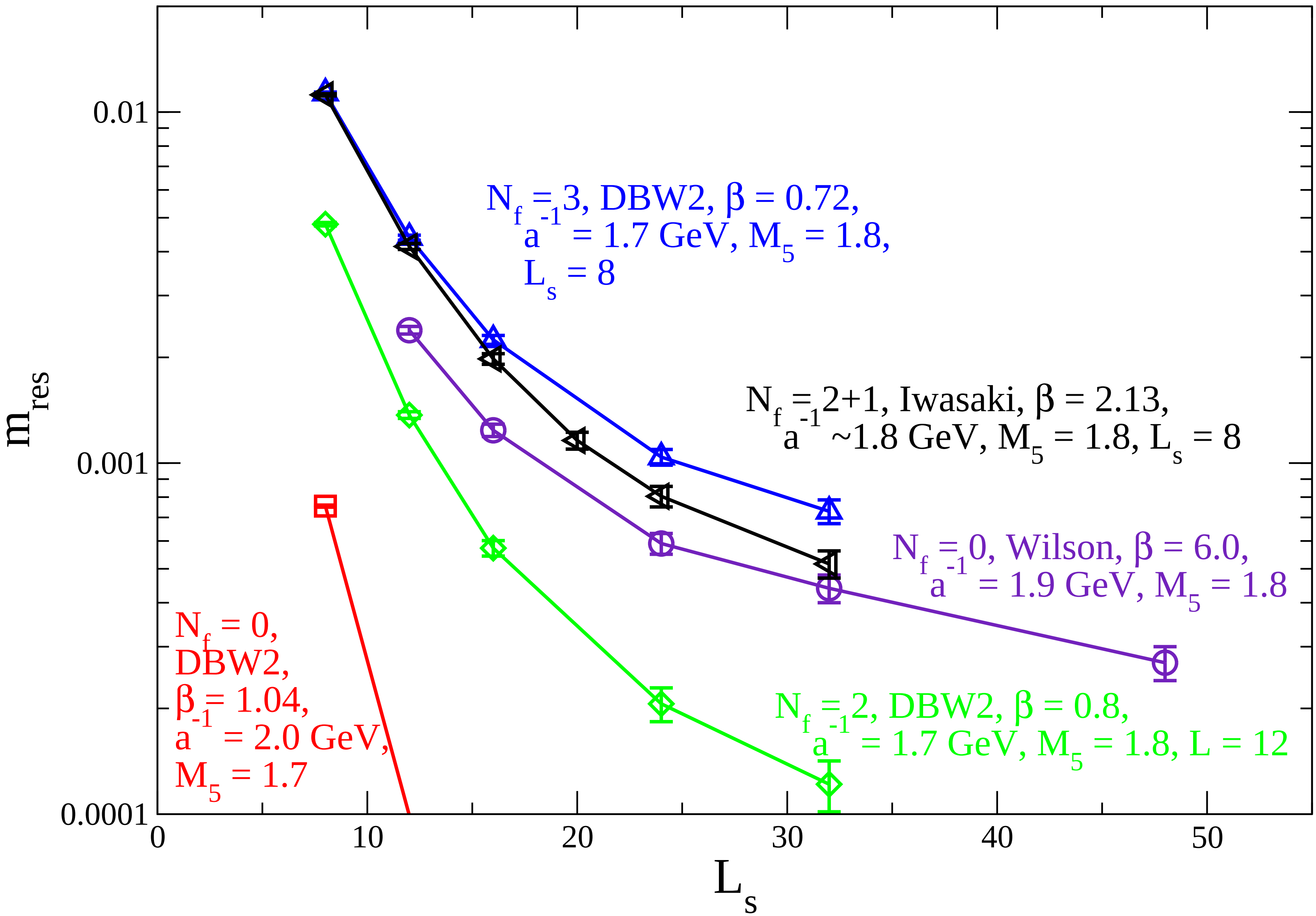


Full QCD with Plaquette plus Rectangle Actions

- Need lines of constant lattice spacing, a, to compare $m_{\rm res}$ at fixed a.
- $N_f = 0$, $a^{-1} = 2$ GeV points nicely fit by $\beta_R/\beta_P = -0.125 + a_1\beta + a_2\beta^2$.
- Used this form to propose $N_f = 3$ DBW2 values.

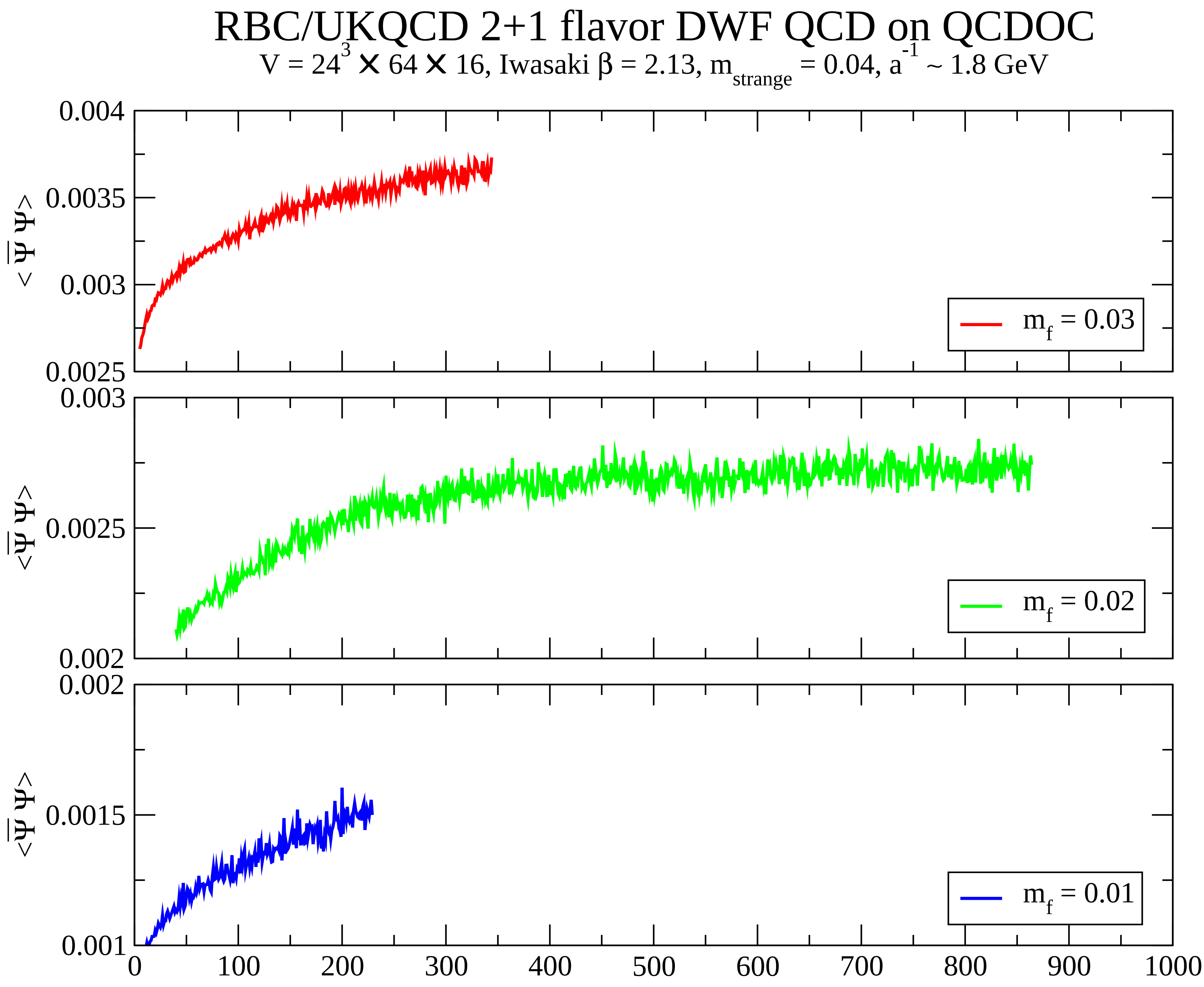


Revisiting $m_{\rm res}$ versus L_s for $N_f = 0, 2$ and 3



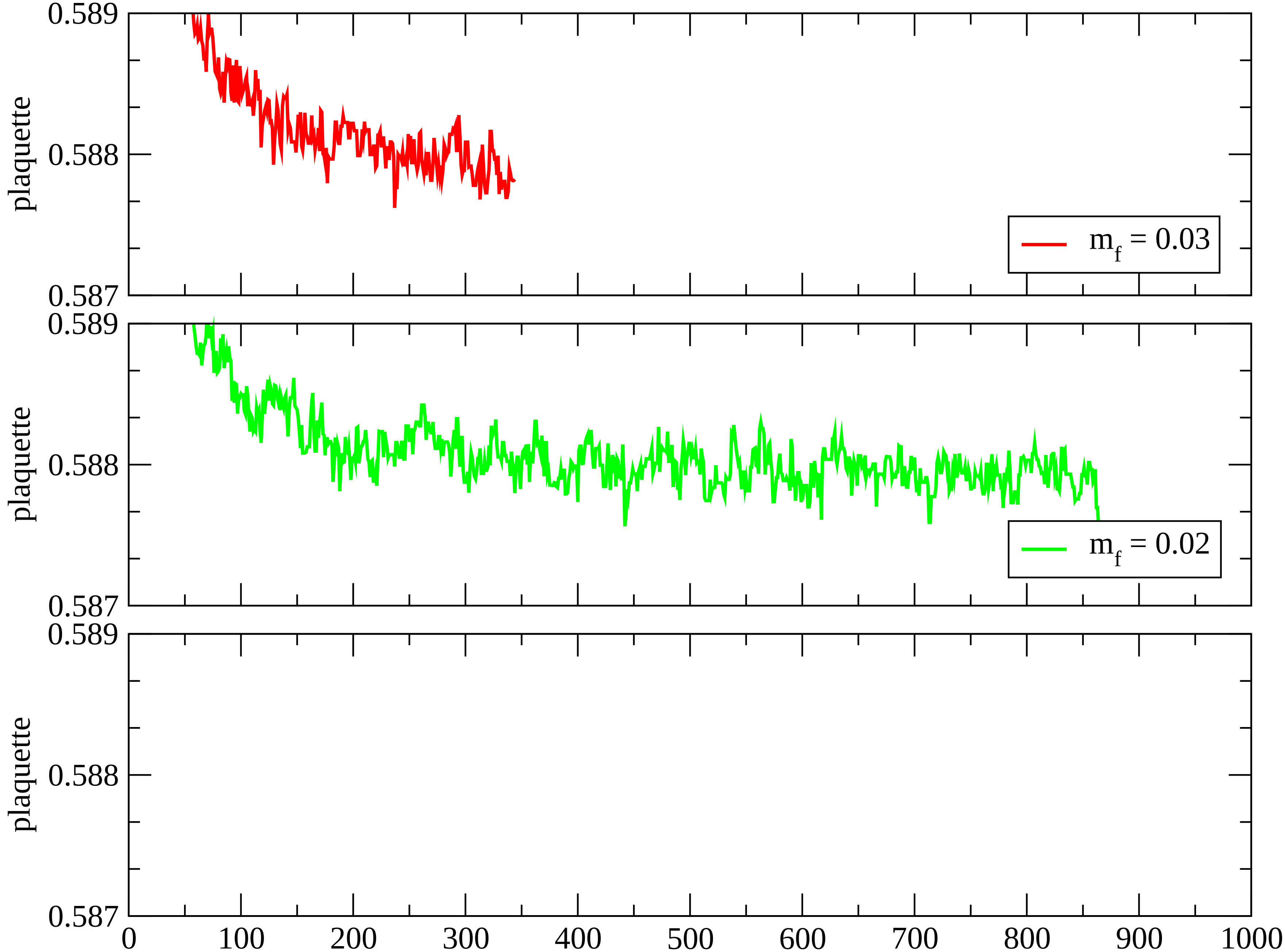
RBC Physics Program -Two Primary Calculations

- 2+1 flavor $T = 0$ DWF using Rational HMC (RHMC) (with UKQCD)
  - Gauge action tests on $16^3 \times 32 \times 8$ - completed
  - Has led to $24^3 \times 64 \times 16$ calculation with $a^{-1} \approx 1.8$ GeV and 2.6 fm box.
  - 5,000 trajectories on $24^3 \times 64 \times 16$ $m_u = m_d \approx m_s/4$ takes 1 year on 4k nodes. ($2\times$ uncertainty)
  - Smaller volume and coarser lattice spacing runs likely done by RBC on USDOE QCDOC.
- 2+1 flavor thermodynamics with P4 staggered fermions (with Bielefeld)
  - P4 has better approach to Stefan-Boltzman limit (Heller, Karsch).
  - Zero temperature scaling study of P4 needed.
  - Do state of art determination of T_c with P4.
  - Continue to investigate thermodynamics with DWF.


RBC/UKQCD 2+1 flavor DWF QCD on QCDOC
V = 24^3 × 64 × 16, Iwasaki β = 2.13, m_strange = 0.04, a^-1 ~ 1.8 GeV
0.004
0.0035
0.003
0.0025
0.002
0.0015
0.001
<Ψ̄ Ψ>
m_f = 0.03
m_f = 0.02
m_f = 0.01
0
100
200
300
400
500
600
700
800
900
1000

RBC/UKQCD 2+1 flavor DWF QCD on QCDOC

$V = 24^3 \times 64 \times 16$, Iwasaki $\beta = 2.13$, $m_{strange} = 0.04$, $a^{-1} \sim 1.8$ GeV



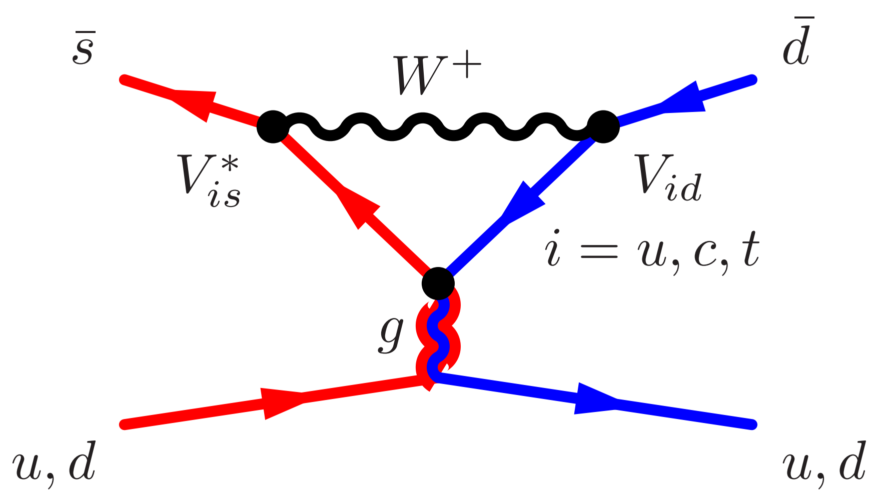
CP Violation in the Standard Model

Imaginary part for $K \to \pi\pi$ amplitudes comes from Cabbibo-Kobayashi-Maskawa (CKM) matrix, which relates quark electroweak eigenstates and quark mass eigenstates

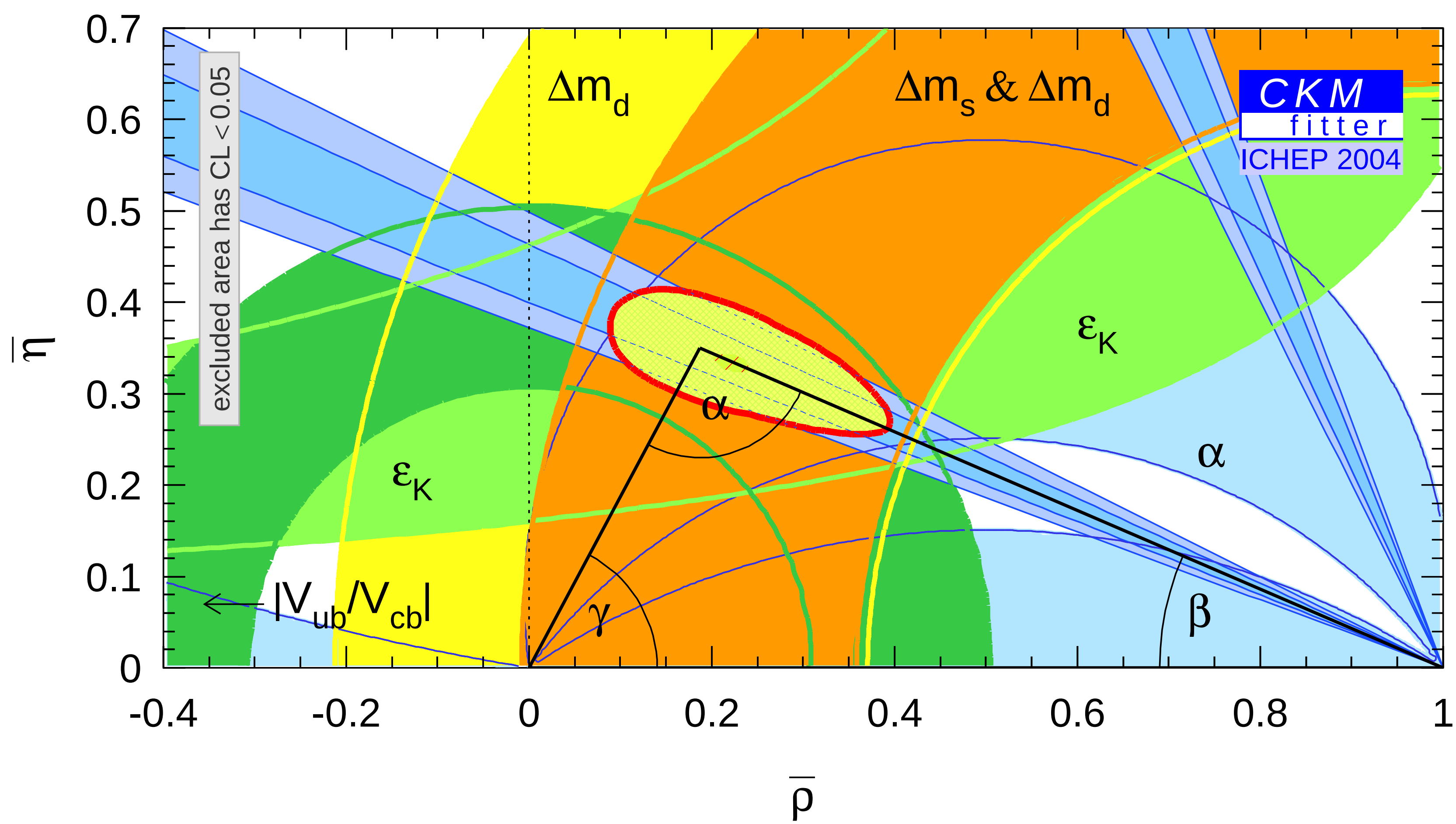
$$\begin{pmatrix} V_{ud} & V_{us} & V_{ub} \\ V_{cd} & V_{cs} & V_{cb} \\ V_{td} & V_{ts} & V_{tb} \end{pmatrix}$$

V_{us} is essentially $\sin\theta_C$, where θ_C is the Cabbibo angle.

V_{ub} and V_{td} are complex. V_{td} effects $K \to \pi\pi$ through "penguin" diagrams.



Unitarity Triangle



CP Violation in the Kaon System

- Two amplitudes determine ϵ and ϵ'

$$\eta_{+-} = \frac{A(K_L^0 \to \pi^+\pi^-)}{A(K_S^0 \to \pi^+\pi^-)} = \epsilon + \epsilon' \qquad \eta_{00} = \frac{A(K_L^0 \to \pi^0\pi^0)}{A(K_S^0 \to \pi^0\pi^0)} = \epsilon - 2\epsilon'$$

- SM: $\overline{K}^0 - K^0$ mixing via $Q^{(\Delta S=2)} = (\bar{s}_\alpha d_\alpha)_{V-A}\,(\bar{s}_\beta d_\beta)_{V-A}$ defines B_K as;

$$\langle \overline{K}^0 | Q^{(\Delta S=2)}(\mu) | K^0 | \rangle \equiv \frac{8}{3} B_K(\mu) f_K^2 m_K^2$$

- RGI parameter $\hat{B}_K \equiv B_K(\mu)\left[\alpha_s^{(3)}(\mu)\right]^{-2/9}\left[1 + \frac{\alpha_s^{(3)}(\mu)}{4\pi} J_3\right]$ relates SM and ϵ

$$\epsilon = \hat{B}_K\,\mathrm{Im}\lambda_t \frac{G_F^2 f_K^2 m_K M_W^2}{12\sqrt{2}\pi^2 \Delta M_K}\left\{\mathrm{Re}\lambda_c\left[\eta_1 S_0(x_c) - \eta_3 S_0(x_c, x_t)\right] - \mathrm{Re}\lambda_t\,\eta_2 S_0(x_t)\right\}\exp(i\pi/4)$$

- Defining $A(K^0 \to \pi\pi(I)) \equiv A_I e^{(i\delta_I)}$, $P_2 \equiv \mathrm{Im}A_2/\mathrm{ReA}_2$, $P_0 \equiv \mathrm{Im}A_0/\mathrm{ReA}_0$:

$$\epsilon' = \frac{ie^{i(\delta_2-\delta_0)}}{\sqrt{2}}\left(\frac{\mathrm{Re}\,A_2}{\mathrm{Re}\,A_0}\right)\left(\frac{\mathrm{Im}\,A_2}{\mathrm{Re}\,A_2} - \frac{\mathrm{Im}\,A_0}{\mathrm{Re}\,A_0}\right) \qquad w \equiv \frac{\mathrm{Re}\,A_0}{\mathrm{Re}\,A_2} \approx 22$$

Operator Mixing and Chiral Symmetry

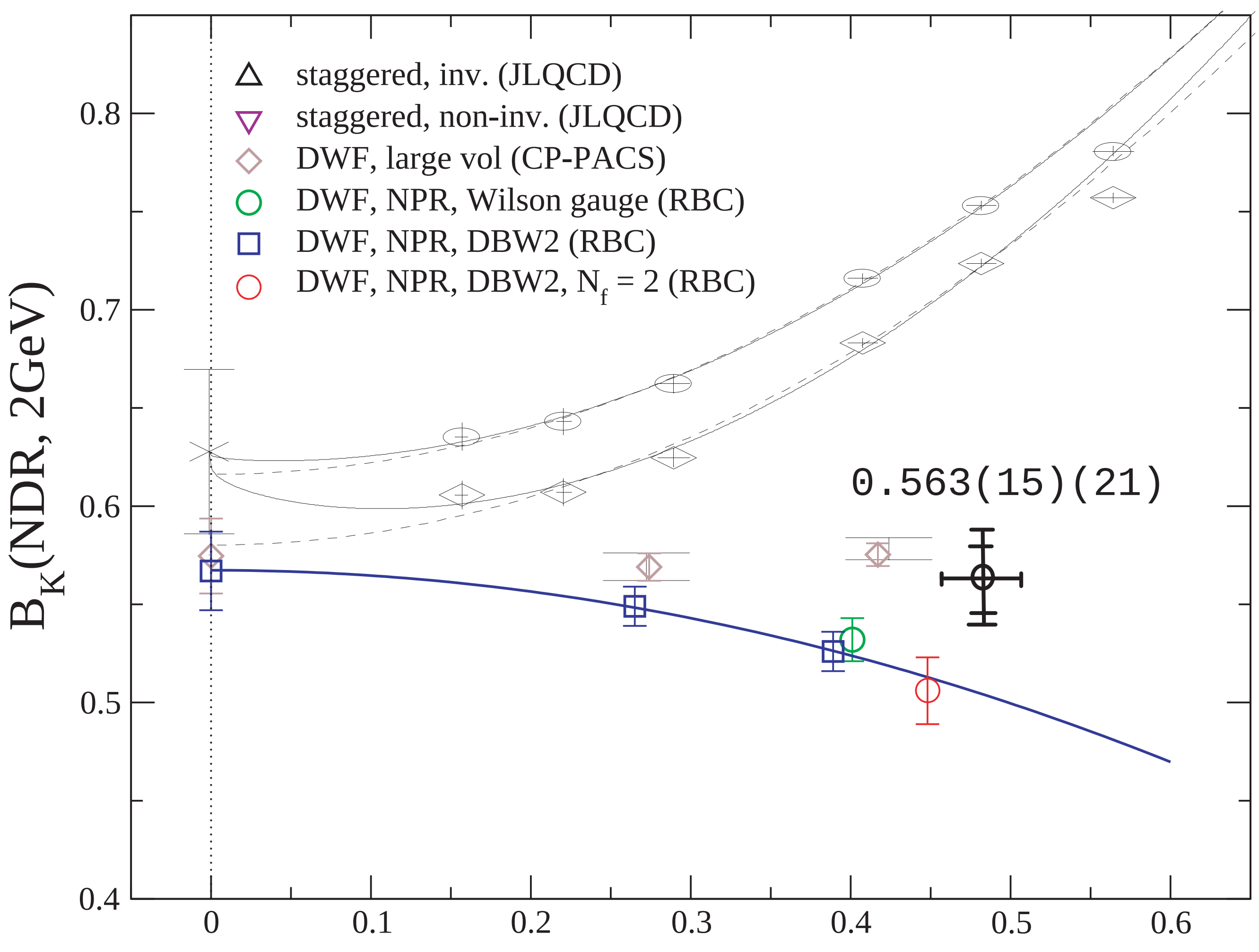
- Presence of lattice chiral symmetry markedly helps operator mixing
- Consider $Q^{(\Delta S=2)}$ as an example

$$
\begin{aligned}
\bar{s}^{\rm lat}\gamma_\mu(1-\gamma_5)d^{\rm lat}\ \bar{s}^{\rm lat}\gamma_\mu(1-\gamma_5)d^{\rm lat} &\equiv (\bar{s}^{\rm lat}d^{\rm lat})_{V-A}\ (\bar{s}^{\rm lat}d^{\rm lat})_{V-A} \\
&= Z_1(\mu a)(\bar{s}d)_{V-A}\ (\bar{s}d)_{V-A} \\
&+ Z_2(\mu a)(\bar{s}d)_{V+A}\ (\bar{s}d)_{V+A} \\
&+ Z_3(\mu a)(\bar{s}d)_{P-S}\ (\bar{s}d)_{P-S} \\
&+ Z_4(\mu a)(\bar{s}d)_{P+S}\ (\bar{s}d)_{P+S} \\
&+ Z_5(\mu a)(\bar{s}d)_{T}\ (\bar{s}d)_{T}
\end{aligned}
$$

- For DWF, Z_2, Z_3, Z_4, Z_5 are $\mathcal{O}(m_{\rm res}^2)$, so small
- For DWF, use non-perturbative renormalization (NPR) (Rome-Southampton)
- Only reliance on continuum perturbation theory in OPE

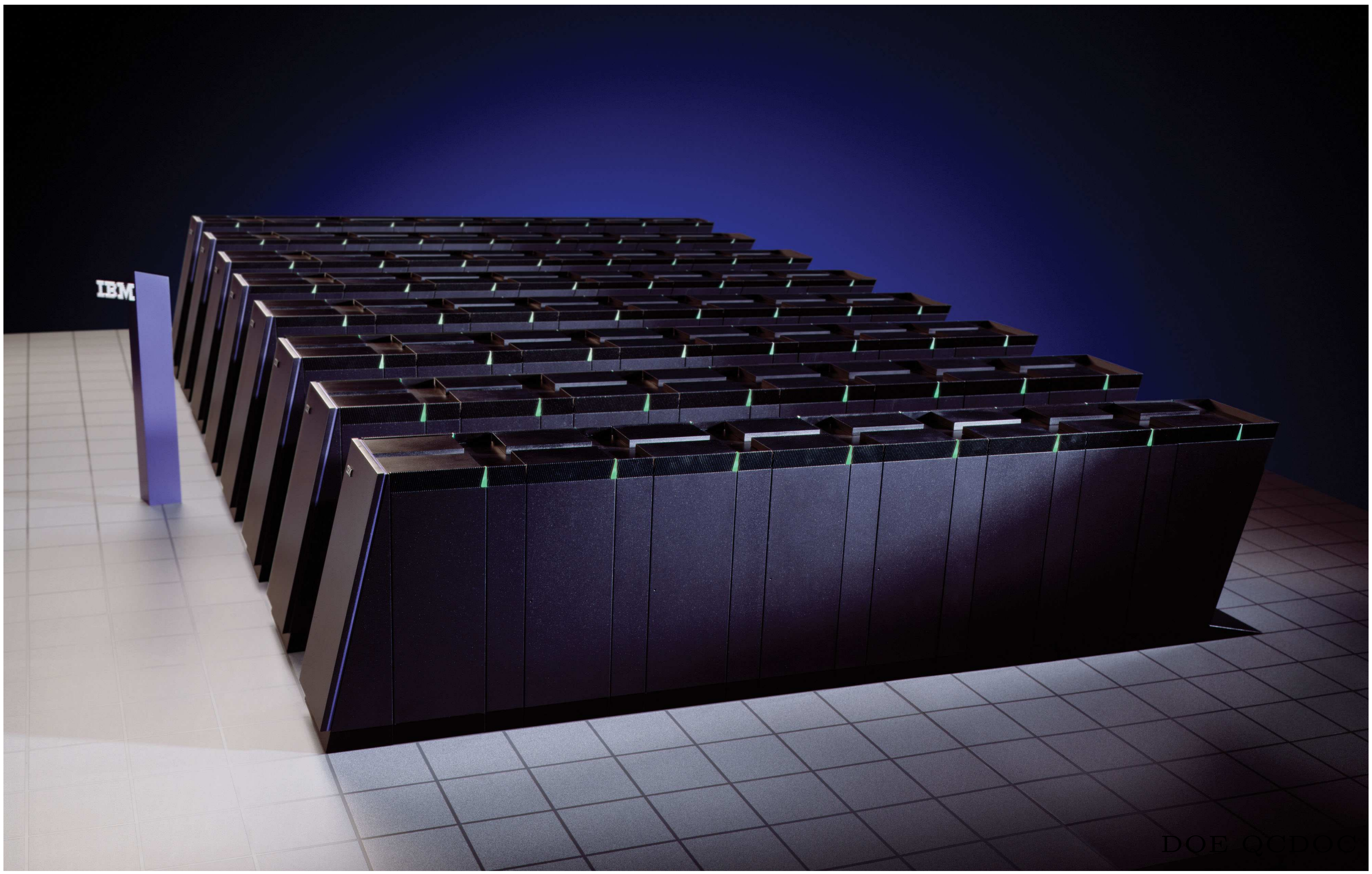
The Kaon B Parameter, $B_K^{\overline{\mathrm{MS}}}(\mu = 2\ \mathrm{GeV})$

	quenched $a \to 0$			dyn. $a^{-1} = 1.7$ GeV
PDG	JLQCD (stag)	CP-PACS (DWF)	RBC (DWF)	RBC (2f DWF)
0.65 ± 0.15	0.628 ± 0.042	0.575 ± 0.019	0.563 ± 0.021 $\pm 39 \pm 30$	0.492 ± 0.018



IBM BlueGene/L

- 3-dimensional mesh architecture, similar to QCDSP and QCDOC
- 65,000 node, 360 TFlops installation at Livermore
- Al Gara is primary architect.



Conclusions, Outlook, and Thanks

- QCDOC provides powerful resource for Lattice QCD.
- BNL ITD staff have assembled and debugged 39, 1,024 node racks of QCDOC since September, 2004. Thanks to Ed McFadden, Ed Brosnan, Joe DePace, Don Gates, Paul Poleski, Andy Como.
- BNL has provided $1.6M in lab funds to renovate space for QCDOC.
- QCDOC is current status of 20+ years of QCD computer projects at Columbia, led by Norman Christ.
- Culmination of long term committment by USDOE.
- For QCDOC, vital contribution of funding and personnel from RIKEN/RBRC and UKQCD
- 2+1 flavor DWF QCD is the real theory - no theoretical shortcuts involved. B_K is example of theoretically well-understood quantity limited only by computer power.
- Some QCDOC time for new ideas!